

# PLASTIC DEFORMATION ASSOCIATED WITH VOID GROWTH: MULTISCALE MODELING

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The nucleation and growth of voids is important in the initial phase of fracture of ductile metals at the microscopic level. We use multiscale modeling to investigate this void growth in dynamic fracture with an emphasis on the concomitant plastic deformation. In this talk we contrast the mechanisms of plasticity and void growth in FCC (copper) and BCC (tantalum and molybdenum) using atomistics, both conventional molecular dynamics and a concurrent multiscale modeling generalization called Coarse-Grained Molecular Dynamics. The latter technique embeds the atomistic model in a generalized finite element model which runs concurrently to capture the long range elastic fields. This minimizes the finite size effects associated with dislocations interacting with the periodic image of the deformed material. The atomistic simulations are used to characterize the dislocation activity in the plastic zone surrounding voids growing under tensile loading. The plasticity and void growth behavior is contrasted among the different types of metals under an array of conditions. The results are compared with on-going dynamic fracture experiments at the LLNL gas gun facility.

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## References

- [1] J. Belak, "On the nucleation and growth of voids at high strain-rates," *J. Comp.-Aided Mater. Design* v. 5, p. 193, (1998).
- [2] R.E. Rudd and J. Belak, "Void Nucleation and Associated Plasticity in Dynamic Fracture of Polycrystalline Copper: An atomistic simulation," *Comput. Mater. Sci.* v. 24, p. 148-153, (2002).